

# Charging effects in the ac conductance of a double barrier resonant tunneling structure

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## Abstract

There have been many studies of the linear response ac conductance of a double barrier resonant tunneling structure (DBRTS). While these studies are important, they fail to self-consistently include the effect of time dependent charge density in the well. In this paper, we calculate the ac conductance by including the effect of time dependent charge density in the well in a self-consistent manner. The charge density in the well contributes to both the flow of displacement currents and the time dependent potential in the well. We find that including these effects can make a significant difference to the ac conductance and the total ac current is not equal to the average of non-selfconsistently calculated conduction currents in the two contacts, an often made assumption. This is illustrated by comparing the results obtained with and without the effect of the time dependent charge density included properly.

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## I. INTRODUCTION

Double-barrier resonant tunneling structures (DBRTS) have been of interest because of possible device applications in building logic circuits, oscillators, detectors etc., and it has much to offer in the study of physics of confined structures. The dc characteristics have been studied extensively by including effects of charging and inelastic scattering. Reference [1] offers a comprehensive review of applications and basic physics of DBRTS. In comparison, there are only a few studies of ac response over various frequencies regimes [2–7]. While some of these studies are based on simulating a realistic device using detailed numerical procedures [2,3], others are based on simple models [4–7]. These calculations however do not include the effect of time varying charge density in the well, which is important in determining ac conductance [3,4,8–11]. Reference [8] has discussed the pitfalls of many existing ac conductance theories qualitatively and reference [9] formulated the theory of ac conductance in the linear response and low frequency regime as applicable to mesoscopic structures by including effects of charging. Subsequently, reference [12] used a non-equilibrium greens function approach to provide a formulation that can be used at finite biases and large frequencies including effects of charging in the well and phonon scattering [13]. The effect of time dependent charge density in the well is of importance in determining the dynamics because electrons in the well image to the outside world, which includes the contacts. This causes flow of displacement currents and contributes to the ac potential in the well. The role of these factors in determining the ac conductance of a DBRTS is not clear from previous work. In this paper, we study the ac conductance of a DBRTS with the aim of illustrating the role of imaging of well-charge to contacts via a simple model. Imaging of well-charge to the two contacts is modeled by capacitances denoted by  $C_1$  and  $C_2$  (figure 1). We would like to clarify at the outset that the purpose of this study

is to illustrate the importance of imaging and not to model a typical resonant tunneling device whose structure is considerably more complicated.

We derive useful expressions for the ac conductance and show that the ac conductance depends significantly on both (i) the ratio of capacitances  $\frac{C_1}{C}$  and  $\frac{C_2}{C}$ , where  $C = C_1 + C_2$  and (ii) the value of the total capacitance between well and contacts. The first feature follows because a time dependent well-charge  $q(t)$  contributes to flow of displacement currents equal to  $\frac{C_1}{C} \frac{dq(t)}{dt}$  and  $\frac{C_2}{C} \frac{dq(t)}{dt}$  in contacts 1 and 2 respectively (figure 1), where  $q(t)$  is charge in the well at time  $t$ . The second feature can be understood by noting that time dependent charge density in the well contributes to ac potential of the well via a term  $\frac{q(t)}{C}$  (figure 1). This affects the current because the ac potential in the well plays a role in determining both the conduction and displacement currents. Note that there is nothing quantum mechanical about these two features and they would be true even if  $C_1$  and  $C_2$  are leaky capacitors in a classical circuit. Quantum mechanics plays a role only in determining the values of  $q(t)$  and current.

Some previous papers calculated the ac conductance of a DBRTS by the following procedure (see section III). The conduction currents across the two barriers are calculated by neglecting the contribution to ac potential in the well from the time dependent charge density. Then the total ac current is taken to be the average of the conduction currents flowing across the two barriers. *We find such a procedure to be valid only when the capacitances are symmetrical ( $C_1 = C_2$ ) and the value of  $C$  is large.*

The remainder of the paper is arranged as follows. In section II, we explain the model adopted in detail. In section III, we discuss the effect of charging on the ac conductance using expressions derived in section II B. In section IV, we discuss the effect of charging on the ac conductance using numerical examples. The effect of including asymmetries in the barrier strengths and the capacitances of an otherwise symmetric structure are systematically studied here. We present

our conclusions in section V.

## II. MODEL

### A. Hamiltonian

We model the resonant tunneling structure by using a tight binding Hamiltonian [4–7,14,15]. The well is represented by a single node with a resonant level at energy  $\epsilon_r$  and is coupled to contacts 1 and 2 (figure 1). The Hamiltonian of the structure is,

$$H = H_D + H_C + H_{CD} \quad (2.1)$$

where,  $H_D = \epsilon_r(t)d^\dagger d$

$$H_C = \sum_{i, \alpha \in 1, 2} (\epsilon_{i\alpha} + ev_1^{ac} \cos(\omega t) \delta_{1,\alpha}) c_{i\alpha}^\dagger c_{i\alpha} + (wc_{i\alpha}^\dagger c_{i+1\alpha} + c.c.)$$

$$H_{CD} = \sum_{\alpha \in 1, 2} w_\alpha c_{0\alpha}^\dagger d + c.c. .$$

We assume that the ac potential is applied only to contact 1.  $d$  ( $d^\dagger$ ) and  $c_{i\alpha}$  ( $c_{i\alpha}^\dagger$ ) are annihilation (creation) operators for electrons in the well and various lattice sites of contact  $\alpha$  respectively. The sites in a contact are labeled starting from 0 which represents the lattice site immediately neighboring the well.  $w_1$  and  $w_2$  represent the coupling between the well and site 0 of contacts 1 and 2 respectively.  $w$  represents the coupling between nearest neighbors in the tight binding lattice of the contacts.  $H_D$ ,  $H_C$  and  $H_{CD}$  represent the Hamiltonians of the isolated well, contacts and coupling between the well and contacts respectively. In the presence of a dc bias  $V_\alpha^{dc}$  applied to contact  $\alpha$ , the on-site potential in contact  $\alpha$  increases by the dc bias ( $\epsilon_{i\alpha} \rightarrow \epsilon_{i\alpha} + eV_\alpha^{dc}$ ). The expression for  $\epsilon_r(t)$  is,

$$\epsilon_r(t) = \epsilon_{r0} + \beta_2 e V_{dc} + \alpha_2 e v_1^{ac}(t) + e V_w^Q(t), \quad (2.2)$$

where,  $\epsilon_{r0}$  is the energy of the resonant level at zero dc and ac biases.  $V_{dc}$  and  $v_1^{ac}$  are dc and ac biases applied to contact 1.  $\beta_2$  and  $\alpha_2$  are fractional drops of the external dc and ac potentials between contact 2 and the well respectively, in absence of charge in the well. The last term of equation (2.2) represents the effect of imaging of charge in the well. The electrons in the well image to the contacts and this is modeled by capacitances  $C_1$  and  $C_2$  (figure 1), which are assumed to be known parameters [9,14]. As a consequence of imaging of well charge, the band bottom in the well (and hence the resonant level) changes by  $V_w^Q(t)$ ,

$$V_w^Q(t) = \frac{q(t)}{C} = V_w^{dc} + v_w^{ac}(t), \quad (2.3)$$

$$\text{where, } V_w^{dc} = \frac{q_{dc}(V)}{C} \quad \text{and} \quad v_w^{ac}(t) = \frac{q(t) - q_{dc}(V)}{C}. \quad (2.4)$$

$q_{dc}(V)$  represents the dc charge in the well when the applied dc voltage is  $V$ .  $q(t)$  is the total charge in the well and  $q(t) - q_{dc}(V)$  is the time dependent component. The total capacitance between the well and contacts is  $C$  ( $= C_1 + C_2$ ).

The total potential of the well  $V_w(t)$  is,

$$V_w(t) = V_w^Q(t) + \beta_2 V_{dc} + \alpha_2 v_1^{ac}(t). \quad (2.5)$$

The first, second and third terms represent the potentials due to imaging of well charge, the externally applied dc and ac potentials respectively.

## B. ac Conductance

The applied ac voltage results in a time dependent well charge that images to the contacts. This (i) causes a flow of displacement currents and (ii) contributes to the time dependent potential of the well ( $V_w^Q$  of equation (2.3)). (ii) plays a role in determining the correct conduction currents. The conduction current is in turn related to the time varying well charge by continuity equation.

In the following discussion, we first define a conductance matrix,  $g$ . The conduction and displacement currents are then expressed in terms of the elements of the conductance matrix. The procedure to evaluate the conductance matrix is discussed in the next subsection.

**The conductance matrix ( $g$ ):** The conductance matrix element  $g_{\alpha\beta}$  represents the ratio of conduction current ( $i_\alpha^c$ ) flowing in contact  $\alpha$  as a result of an ac voltage ( $v_\beta$ ) applied to contact  $\beta$ , with the ac potential in well and contacts set equal to zero:

$$g_{\alpha\beta}(\omega) = \frac{i_\alpha^c(\omega)}{v_\beta^{ac}(\omega)}, \text{ where } \alpha, \beta \in 1, 2. \quad (2.6)$$

The dc voltage is set to its steady state value, i.e., the dc component of equation (2.5).

**Conduction current:** Consider an ac potential  $v_1^{ac}$  applied to contact 1, with contact 2 grounded. As a result, the potential of the well develops a time dependent component,  $v_w(\omega)$  (equation (2.5) [16]). The linear response ac current flowing in contact  $i \in 1, 2$  consists of two terms (i) due to ac potential  $v_1^{ac}$ , with ac potentials in the well and contact 2 set equal to zero and (ii) due to ac potential  $v_w(\omega)$  in the well, with ac potential in contacts 1 and 2 set equal to zero. The first component is  $g_{i1}v_1^{ac}$ . This follows from the definition in equation (2.6). The second component is physically equivalent to setting the ac potential in the well equal to zero along with an ac potential  $-v_w(\omega)$  applied to contacts 1 and 2. The linear response current flowing in contact  $i$  due to this component is  $-(g_{i1} + g_{i2})v_w(\omega)$  (from equation (2.6)). The total ac conduction current flowing in contacts 1 and 2 is the sum of the two components,

$$\begin{aligned} \text{ac conduction current in contact 1} &= g_{11}(\omega)(v_1^{ac}(\omega) - v_w(\omega)) + g_{12}(\omega)(-v_w(\omega)) \\ \text{ac conduction current in contact 2} &= g_{21}(\omega)(v_1^{ac}(\omega) - v_w(\omega)) + g_{22}(\omega)(-v_w(\omega)) . \end{aligned} \quad (2.7)$$

Now, if external ac potentials  $v_1^{ac}(\omega)$  and  $v_2^{ac}(\omega)$  are applied to both contacts 1 and 2, then the conduction current in the two contacts is given by,

$$I_1^c(\omega) = g_{11}(\omega)(v_1^{ac}(\omega) - v_w(\omega)) + g_{12}(\omega)(v_2^{ac}(\omega) - v_w(\omega)) \quad (2.8)$$

$$I_2^c(\omega) = g_{21}(\omega)(v_1^{ac}(\omega) - v_w(\omega)) + g_{22}(\omega)(v_2^{ac}(\omega) - v_w(\omega)) . \quad (2.9)$$

The well charge is related to the conduction currents by the continuity equation,

$$\frac{dq(t)}{dt} = I_1^c(t) + I_2^c(t) \implies q(\omega) = \frac{I_1^c(\omega) + I_2^c(\omega)}{-j\omega} . \quad (2.10)$$

Substituting equation (2.10) in equations (2.3) and (2.5), the ac potential of the device can be written as,

$$v_w(\omega) = \alpha_2 v_1^{ac}(\omega) + \frac{I_1^c(\omega) + I_2^c(\omega)}{-j\omega C} . \quad (2.11)$$

Using equations (2.8), (2.9) and (2.11), the conduction currents in contacts 1 and 2 can be expressed in terms of the  $g$  matrix elements:

$$G_1^c(\omega) = \frac{I_1^c(\omega)}{v_1^{ac}} = + \frac{\alpha_1 g_{11} - \alpha_2 g_{12} + \frac{1}{-j\omega C}(g_{11}g_{22} - g_{12}g_{21})}{1 + \frac{1}{-j\omega C}(g_{11} + g_{22} + g_{12} + g_{21})} , \quad (2.12)$$

$$G_2^c(\omega) = \frac{I_2^c(\omega)}{v_1^{ac}} = - \frac{\alpha_2 g_{22} - \alpha_1 g_{21} + \frac{1}{-j\omega C}(g_{11}g_{22} - g_{12}g_{21})}{1 + \frac{1}{-j\omega C}(g_{11} + g_{22} + g_{12} + g_{21})} . \quad (2.13)$$

Here  $\alpha_1$  and  $\alpha_2$  are fractional drops in the externally applied ac potential between the well and contacts 1 and 2 respectively, in absence of charge in the well.

**Displacement Current:** The displacement current flowing in contact  $\alpha$  consists of two components. One component  $\pm j\omega C$  (the plus and minus signs are for the currents in the two different contacts) is due to the dielectric nature of the barrier and well. This component does not depend on tunneling of charge from the contacts to well and is not explicitly written in the remainder of the paper. The other component, which is due to tunneling of charge from the contacts to well, is equal to  $j\omega \frac{C_\alpha}{C}$ . The total displacement current in the two contacts are given by,

$$I_1^d(\omega) = j\omega \frac{C_1}{C} q(\omega) = -\frac{C_1}{C} (I_1^c(\omega) + I_2^c(\omega)) \quad (2.14)$$

$$I_2^d(\omega) = j\omega \frac{C_2}{C} q(\omega) = -\frac{C_2}{C} (I_1^c(\omega) + I_2^c(\omega)) . \quad (2.15)$$

Solving equations (2.8)-(2.15), we get the following expression for conductance contributions from conduction and displacement currents:

$$G_\alpha^d(\omega) = \frac{I_\alpha^d(\omega)}{v_1^{ac}} = \frac{C_\alpha}{C} \frac{\alpha_1(g_{11} + g_{21}) - \alpha_2(g_{22} + g_{12})}{1 + \frac{1}{-j\omega C}(g_{11} + g_{22} + g_{12} + g_{21})}, \quad (2.16)$$

where,  $\alpha = 1, 2$  and  $\omega$  has been suppressed from the arguments of the  $g$  matrix elements.

**Total current:** Using equations (2.14) and (2.15), it can be seen that the total current (conduction plus displacement) in the contacts can be expressed in terms of the conduction currents,

$$I_1(\omega) = I_1^c(\omega) + I_1^d(\omega) = \frac{C_2}{C} I_1^c(\omega) - \frac{C_1}{C} I_2^c(\omega) \quad (2.17)$$

$$\text{and } I_2(\omega) = I_2^c(\omega) + I_2^d(\omega) = \frac{C_1}{C} I_2^c(\omega) - \frac{C_2}{C} I_1^c(\omega) = -I_1(\omega). \quad (2.18)$$

We would like to emphasize that  $I_1^c(\omega)$  and  $I_2^c(\omega)$  are the conduction currents calculated by including the contribution to ac potential in the well due to ac well charge density. In the remainder of the paper it is assumed that  $\alpha_1$  and  $\alpha_2$  are equal to fractional drops in the potentials across  $C_1$  and  $C_2$  (figure 1). Then,  $\alpha_1 = \frac{C_2}{C}$  and  $\alpha_2 = \frac{C_1}{C}$ . Substituting equations (2.12) and (2.13) in equations (2.17) and (2.18), the total ac conductance is:

$$G_1(\omega) = + \frac{\alpha_1^2 g_{11} + \alpha_2^2 g_{22} - \alpha_2 \alpha_1 (g_{12} + g_{21}) + \frac{1}{-j\omega C} (g_{11} g_{22} - g_{12} g_{21})}{1 + \frac{1}{-j\omega C} (g_{11} + g_{22} + g_{12} + g_{21})} \quad (2.19)$$

$$G_2(\omega) = -G_1(\omega). \quad (2.20)$$

### C. Calculation of the Conductance Matrix Elements: $g_{\alpha\beta}$

The general expression for the ac conduction current in contact  $\alpha$  taken from reference [12] are,

$$i_\alpha(\omega) = \frac{e}{\hbar} \int_{-\infty}^{+\infty} \frac{dE}{2\pi} \text{Tr} \{ i_\alpha^{(1)}(E, \omega) + i_\alpha^{(2)}(E, \omega) + i_\alpha^{(3)}(E, \omega) + i_\alpha^{(4)}(E, \omega) \} \quad (2.21)$$

where,

$$i_{\alpha}^{(1)}(E, \omega) = \sigma_{\alpha}^{<}(E + \hbar\omega, E) [ G^r(E + \hbar\omega) - G^a(E) ] \quad (2.22)$$

$$i_{\alpha}^{(2)}(E, \omega) = -j\Gamma_{\alpha}g^{<}(E + \hbar\omega, E) \quad (2.23)$$

$$i_{\alpha}^{(3)}(E, \omega) = g^r(E + \hbar\omega, E)\Sigma_{\alpha}^{<}(E) - g^a(E + \hbar\omega, E)\Sigma_{\alpha}^{<}(E + \hbar\omega) \quad (2.24)$$

$$i_{\alpha}^{(4)}(E, \omega) = \sigma_{\alpha}^r(E + \hbar\omega, E)G^{<}(E) - G^{<}(E + \hbar\omega)\sigma_{\alpha}^a(E + \hbar\omega, E). \quad (2.25)$$

Here the functions represented by capital letters are calculated in the steady state limit and the functions represented by small letters are calculated to first order in the applied ac potential.  $G^r$ ,  $g^r$ ,  $G^a$ , and  $g^a$  are retarded and advanced greens functions at the site representing the well. Similarly  $\Sigma_{\alpha}^r$ ,  $\sigma_{\alpha}^r$ ,  $\Sigma_{\alpha}^a$ , and  $\sigma_{\alpha}^a$  are retarded and advanced self energies at the well site due to coupling with contact  $\alpha$ . The function  $\Sigma_{\alpha}^{<}(E)$  represents injection of electrons from contact  $\alpha$  to device at energy  $E$ .  $\sigma_{\alpha}^{<}(E + \hbar\omega, E)$  represents time-dependent injection from contact  $\alpha$  to device.

Using the expressions for dc [15,17] and ac [12] selfenergies, applying an ac potential to contact  $\beta$  yields,

$$\Sigma_{\alpha}^r(E) = j\Gamma_{\alpha}(E) \quad (2.26)$$

$$\Sigma_{\alpha}^{<}(E) = j\Gamma_{\alpha}(E)f_{\alpha}(E) \quad (2.27)$$

$$\sigma_{\alpha}^r(E + \omega, E) = \frac{\Sigma_{\alpha}^r(E) - \Sigma_{\alpha}^r(E + \omega)}{\omega} \delta_{\alpha\beta} \quad (2.28)$$

$$\sigma_{\alpha}^{<}(E + \omega, E) = \frac{\Sigma_{\alpha}^{<}(E) - \Sigma_{\alpha}^{<}(E + \omega)}{\omega} \delta_{\alpha\beta}, \quad (2.29)$$

where,  $\alpha$  stands for contacts 1 and 2. In the expression for retarded self energy, we only keep the imaginary part and neglect the real part which represents a shift in the resonant energy [17].

In the dc limit the expression for  $\Gamma_{\alpha}(E)$  is [18],

$$\Gamma_{\alpha}(E) = \frac{w_{\alpha}^2}{w} \sin(k_{\alpha}a) \quad \text{for } E > V_{\alpha} \quad (2.30)$$

$$\Gamma_{\alpha}(E) = 0 \quad \text{for } E < V_{\alpha}. \quad (2.31)$$

Due to absence of inter-mode scattering, the greens functions take the following

form (using expressions for  $g$  and  $G$  from references [12] and [15] respectively):

$$G^r(E) = \frac{1}{E - \epsilon_{r0} + \Sigma(E)} \quad (2.32)$$

$$G^<(E) = G^r(E)\Sigma^<(E)G^a(E) \quad (2.33)$$

$$g^r(E + \omega, E) = G^r(E + \omega)\sigma^r(E + \omega, E)G^r(E) \quad (2.34)$$

$$\begin{aligned} g^<(E + \omega, E) = & G^r(E + \omega)\sigma^<(E + \omega, E)G^a(E) + \\ & g^r(E + \omega, E)\Sigma^<(E)G^a(E) + \\ & G^r(E + \omega)\Sigma^<(E + \omega)g^a(E + \omega, E) \}. \end{aligned} \quad (2.35)$$

Using equations (2.26)-(2.29) and equations (2.32)-(2.35) in equation (2.21), the various conductance matrix elements are calculated.

### III. EFFECT OF CHARGING ON THE AC CURRENT

Many references calculate the ac current by neglecting the effect of charging in the device [2–7]. Specifically, reference [6] calculates the ac conduction currents flowing in the two contacts by neglecting the effect of charging. It is then asserted that the total ac current is equal to the average of calculated conduction currents in the two contacts:

$$I(\omega) = \frac{1}{2}(i_1^c(\omega) - i_2^c(\omega)), \quad (3.1)$$

where,  $i_1^c(\omega)$  and  $i_2^c(\omega)$  are conduction currents calculated by neglecting charging.

To illustrate the importance of charging and to show that equation (3.1) is valid only under a special circumstance, we summarize our line of argument from the previous section:

The total current is the sum of the conduction and displacement currents,

$$I_1(\omega) = I_1^c(\omega) + I_1^d(\omega)$$

$$\text{and } I_2(\omega) = I_2^c(\omega) + I_2^d(\omega).$$

The conduction currents here should be calculated by including the effect of the potential in the well due to time varying charge density in the well [equation (2.3)]. The displacement currents are related to the time dependent charge density and are given by,

$$I_1^d(\omega) = j\omega \frac{C_1}{C} q(\omega) \text{ and}$$

$$I_2^d(\omega) = j\omega \frac{C_2}{C} q(\omega).$$

Now  $q(\omega)$  in the above equations can be related to the conduction currents using the continuity equation,

$$\frac{dq(t)}{dt} = I_1^c(t) + I_2^c(t) \implies q(\omega) = \frac{I_1^c(\omega) + I_2^c(\omega)}{-j\omega}$$

Using the previous five equations, the total current can be expressed in terms of the conduction currents (calculated by including the effect of charging in the well) as,

$$I_1(\omega) = \frac{C_2}{C} I_1^c(\omega) - \frac{C_1}{C} I_2^c(\omega)$$

$$\text{and } I_2(\omega) = \frac{C_1}{C} I_2^c(\omega) - \frac{C_2}{C} I_1^c(\omega).$$

From these equations, we see that equation (3.1) is an appropriate expression for the conduction current only when both  $C_1 = C_2$  and conduction currents are calculated by neglecting the effect of charging.

In terms of our notation involving the  $g$  matrix elements, equation (3.1) corresponds to the following equation which is obtained by setting  $C = \infty$  and  $C_1 = C_2$  in equation (2.19):

$$G_1(\omega) = -G_2(\omega) = \frac{1}{2} \{ \alpha_1 (g_{11} - g_{21}) + \alpha_2 (g_{22} - g_{12}) \}. \quad (3.2)$$

In section IV, we will numerically compare our results obtained from equation (2.19) to those obtained from equation (3.2).

#### IV. NUMERICAL EXAMPLES

In this section, we demonstrate the effect of charging on the ac conductance by comparing the conductances calculated with and without charging. The values of  $\epsilon_r$ ,  $\Gamma_1$  and  $\Gamma_2$  are chosen only to illustrate the discussion of section III. Capacitances comparable to those used here are possible only in very narrow cross section devices. The discussion of section III is however valid for broad area resonant tunneling devices as well, where the effect of capacitances is equally important. In Example 1, we start with a device which is symmetric both in the barrier strengths and capacitances, at zero bias. Here the conductance calculated from equations (2.19) and (3.2) are comparable. The effect of introducing an asymmetry in only the barriers (Example 2) and the capacitances (Example 3) of the structure in example 1 is then studied. In Example 4, we discuss the ac conductance of a device in the presence of an applied bias. In the numerical examples considered here, we have verified that the low frequency ac conductance is equal to the differential conductance of the dc I-V curve.

**Example 1.** *Symmetric device at zero bias:*

The conductance versus frequency with and without charging [equations (2.19) and (3.2)] are found to be the same (circles and crosses of figure 3). This is because in the limit of a symmetric device at zero bias, the ac charge density in the well is zero (This follows from equations (2.10), (2.12), (2.13) and by noting that for a symmetric structure at zero bias  $g_{ij} = g_{ji}$ ). As a result both the ac potential and the displacement currents due to the charge in the well are zero. The parameters chosen in this example are:  $V_{dc} = 0\text{V}$ , the chemical potential of contact 1 ( $\mu_1$ ) and contact 2 ( $\mu_2$ ) are chosen to be  $10\text{meV}$ ,  $\epsilon_r = 10\text{meV}$ ,  $\Gamma_1 = \Gamma_2 = 0.1\text{meV}$  at  $E = \epsilon_r$ ,  $w = 2000\text{meV}$ ,  $w_1 = w_2 = \frac{w}{16.7}$ ,  $C_1 = C_2 = 2 \times 10^{-16}\text{F}$  and  $kT = 0.015\text{meV}$ .

**Example 2.** *Effect of asymmetry only in the barrier strength:*

The structure is identical to that in Example 1 except that the barriers are asymmetric ( $\Gamma_1 = 0.02\text{meV}$  and  $\Gamma_2 = 0.1\text{meV}$ ). Then, the results predicted by equations (2.19) and (3.2) are comparable [figure 2(a)]. This can be explained as the total capacitance between the device and the contacts is so large that the contribution to the ac potential in the well due to the  $\frac{q(\omega)}{C}$  term in equation (2.3) is negligible and that  $C_1 = C_2$  (see discussion in section III).

In the case of a structure with smaller capacitances ( $C_1 = C_2 = 1 \times 10^{-16}\text{F}$ ), the results obtained from equations (2.19) and (3.2) are different [figure 2(b)]. This is because when the total capacitance is small, the potential of the well is altered significantly by the charge in it. Then, the conduction currents calculated with and without charging included are different. Note that equation (3.2) does not predict a change in the ac conductance when the capacitances are changed without altering the ratios  $\alpha_1$  and  $\alpha_2$  [see the circles and cross marks in figures 3(a) and (b)].

**Example 3.** *Effect of asymmetry only in the capacitances:*

A DBRTS where an asymmetry in the capacitances has been introduced in example 1 ( $C_1 = 1 \times 10^{-15}\text{F}$  and  $C_2 = 5 \times 10^{-15}$ , the barriers are symmetric) is now considered. Here  $C$  is large enough that the  $\frac{q}{C}$  term does not contribute substantially to the ac potential in the well. The answers obtained from equations (2.19) and (3.2) are different (figure 3) because unequal displacement currents flow in the two contacts when  $C_1 \neq C_2$ . Then, a simple averaging of the conduction currents as in equations (3.1) and (3.2) is no longer valid. Note that the answer for the ac conductance from equation (3.2) is identical in examples 1 and 3 because equation (3.2) does not correctly account for the asymmetry in the capacitances.

**Example 4.** *ac conductance in the presence of an applied voltage:*

The dc bias is chosen to be  $V = 5\text{mV}$  for the example in figure 4 and the self-consistently determined position of the resonance is  $10.5362\text{ meV}$ . The values of

the various parameters are  $C_1 = C_2 = 1 \times 10^{-15} \text{F}$ ,  $w = 2000 \text{meV}$ ,  $w_1 = \frac{w}{17.1}$ ,  $w_2 = \frac{E}{17.1}$ ,  $\epsilon_{r0} = 8.0 \text{meV}$ ,  $\mu_1 = 15 \text{meV}$ ,  $\mu_2 = 10 \text{meV}$  and  $kT = 0.037 \text{meV}$ . From figure 4(a), we see that the elements of the  $g$  matrix,  $g_{12}$  and  $g_{22}$  are larger than  $g_{21}$  and  $g_{11}$  respectively. This feature can be understood by noting that the  $g$  matrix elements depend on the variation of the Fermi function in the contacts and that this variation is more rapid around the resonant energy in contact 2 than in contact 1 [equation (2.29)]. Also, the real part of  $g_{12}$  and the imaginary part of  $g_{22}$  exhibit a peak around a frequency of  $0.5 \text{meV}$  because the resonant energy in the well is about  $0.5362 \text{ meV}$  above the chemical potential of contact 2. We are in the regime where the  $\frac{q}{C}$  component of  $V_w$  is negligible and  $C_1 = C_2$ . So the ac conductance here agrees well with that obtained from equation (3.2). From equation (2.19), we find that  $G_1(\omega) = \frac{1}{4}(g_{11} + g_{22} - g_{12} - g_{21})$ . This expression explains why the ac conductance looks similar to  $g_{22}$ , the largest of the  $g$  matrix elements [figure 4(b)].

On the other hand, we know from section III that for a device where  $C_1 \neq C_2$ , the ac conductance depends on the ratio of  $C_1$  and  $C_2$ . To illustrate this, we keep the values of the resonant energy, applied bias and all other parameters the same as those used in figure 4(b), except that  $C_2 = 4C_1 = 4 \times 10^{-15} \text{F}$ . From equation (2.19),  $G_1(\omega) = \frac{16}{25}g_{11} + \frac{1}{25}g_{22} - \frac{4}{25}(g_{12} + g_{21})$ . While the  $g$  matrix elements remain the same as in figure 4, it is obvious from the expression for  $G_1(\omega)$  that the conductance here is very different from the previous case [figure 4(c)]. In contrast, equation (3.2) predicts the same value for the ac conductance in the two cases [19].

**Experiments:** We now make some remarks on the experimental conditions necessary to observe the differences in the ac conductance discussed. Example 1 corresponds to a symmetric GaAs-AlGaAs structure with identical barriers on either side. A structure with equal capacitances between the well and the two

contacts but with different coupling strengths to the contacts (example 2) can be constructed as follows. The coupling across the left barrier can be made weaker by increasing the barrier height. For AlGaAs, the dielectric constant does not change significantly as the Al doping is increased in the left barrier so as to increase the barrier height. As a result, the barriers will have nearly the same width and hence capacitances. With regards to example 3, the capacitance across the second barrier can be made five times larger by making the barrier about five times thinner than the first barrier. To have similar transmission coefficients, the barrier height of the second barrier should be correspondingly increased. These requirements can probably be met with the present advances in band gap engineering and the exact values of the barrier heights and widths are easy to determine. What is more difficult to achieve is the close proximity of the contacts to the barriers that we have assumed in this paper. This assumption was however made only to make the calculations simpler and more realistic calculations that are beyond the scope of the present work can be carried out.

## V. CONCLUSIONS

In this paper, we have calculated the ac conductance of a DBRTS by including the effect of imaging of charge from the well to the two contacts and present useful expressions to calculate the ac conductance of a DBRTS. The formalism is applicable at high frequencies and in the presence of finite dc biases. The self-consistent inclusion of the effect of imaging of well charge is central to calculating total currents which are equal in the two contacts. We find that including the effect of imaging of charge from the well to the contacts plays a significant role in determining the ac conductance of a DBRTS. The time varying charge density in the well contributes to a flow of displacement currents equal to  $\frac{C_1}{C} \frac{dq}{dt}$  and  $\frac{C_2}{C} \frac{dq}{dt}$  in contacts 1 and 2 respectively ( $q(t)$  is the well charge). The strength of imaging

which is modeled by the total capacitance  $C$  plays a role in determining the ac potential in the well via the  $\frac{q(t)}{C}$  term. These features were illustrated using simple numerical examples in section IV. Some previous papers calculated the ac conductance of a DBRTS by the following procedure. The conduction currents across the two barriers are calculated by neglecting the contribution to the ac potential in the well due to imaging of the time dependent charge density. Then the total ac current is taken to be the average of the conduction currents flowing across the two barriers. In conclusion, we have shown that such a procedure to calculate the ac conductance is correct only when both the capacitance is symmetrical ( $C_1 = C_2$ ) and the value of  $C$  is large.

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[19] The position of the resonance is not calculated self-consistently here as we only want to illustrate the effect of changing the capacitances.

**Figure Captions:**

**Figure 1:** (a) Band Structure of a DBRTS. (b) The DBRTS is modeled by the tight binding Hamiltonian. (c) Imaging of charge from the well to the contacts is accounted for by capacitive coupling between the well and the contacts via capacitances  $C_1$  and  $C_2$ .

**Figure 2:** *Asymmetry only in the barrier strengths:* (a) barriers are symmetric and the total capacitance is large. (b) same structure as (a) but the total capacitance is small.

**Figure 3:** *Asymmetry only in the Capacitances*

**Figure 4:** *ac conductance in the presence of an applied bias.* (a) The conductance matrix elements. (b) The total conductance looks similar to the largest conductance matrix element  $g_{22}$  for this structure when  $C_1 = C_2$ . (c) The total conductance for a device where  $C_2 = 4C_1$  is however different from case (b).

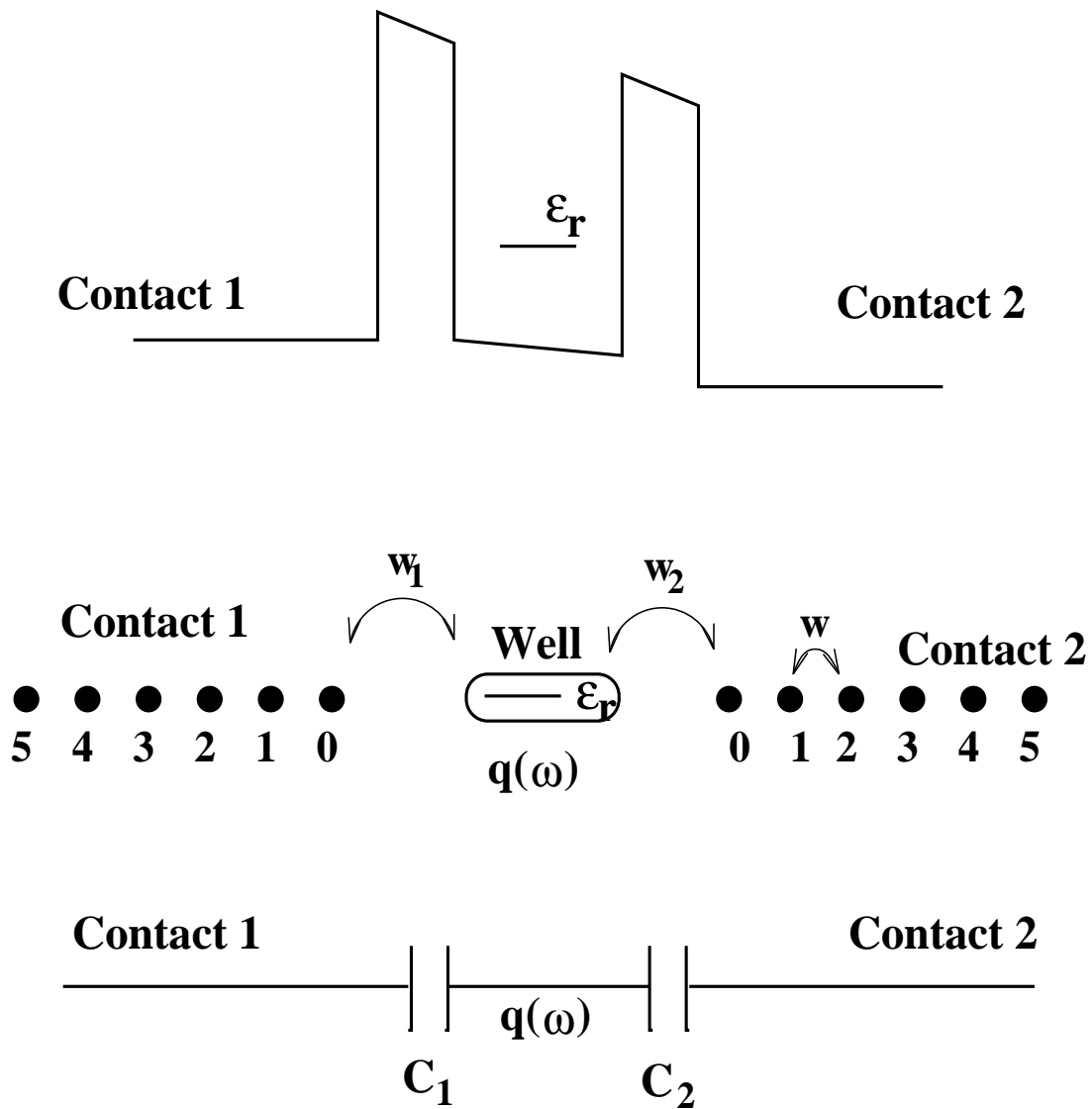


Fig. 1 / Anantram

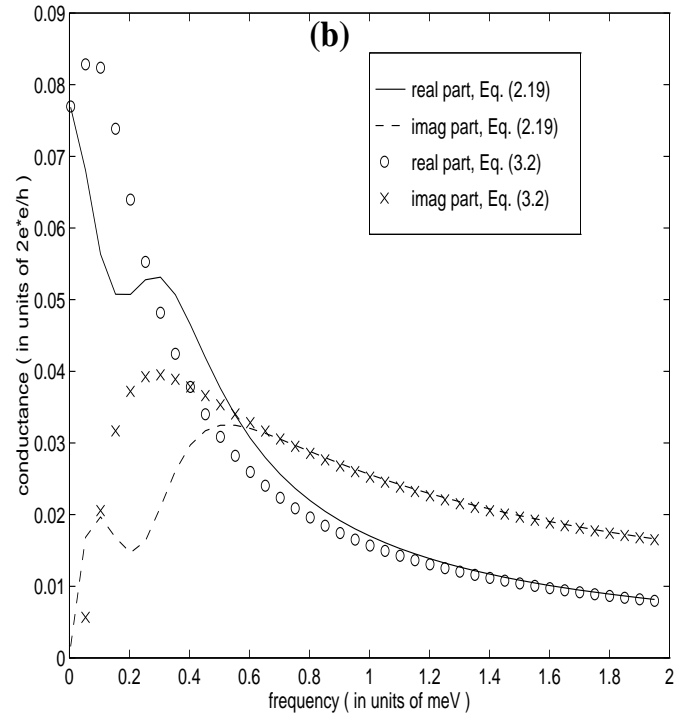
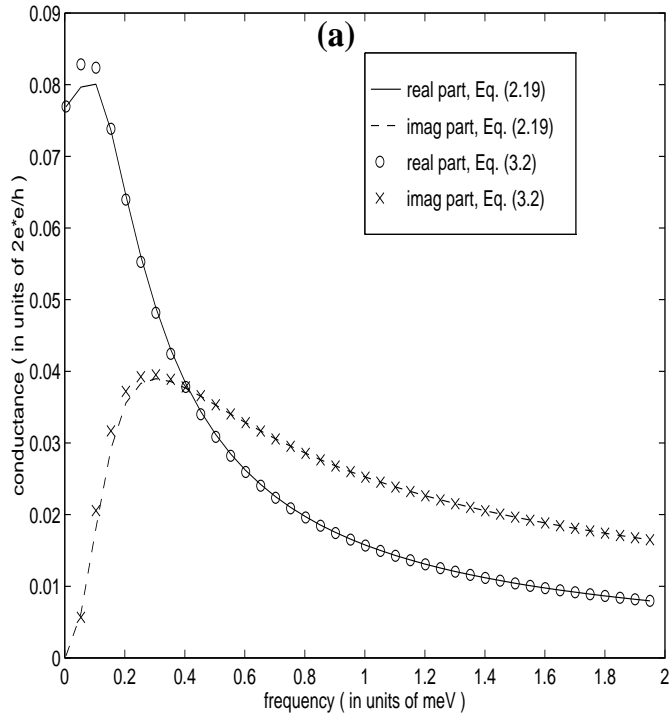


Fig. 2 / Anantram

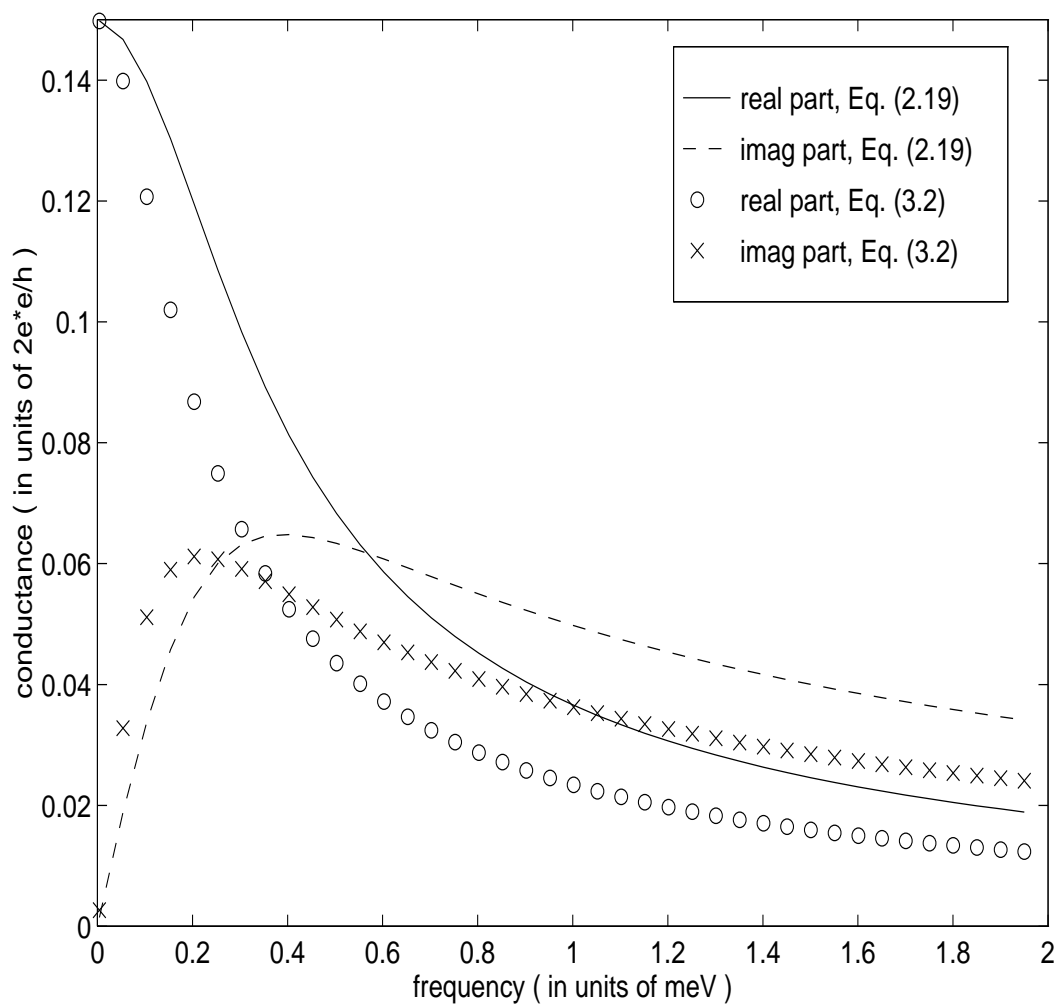


Fig. 3 / Anantram

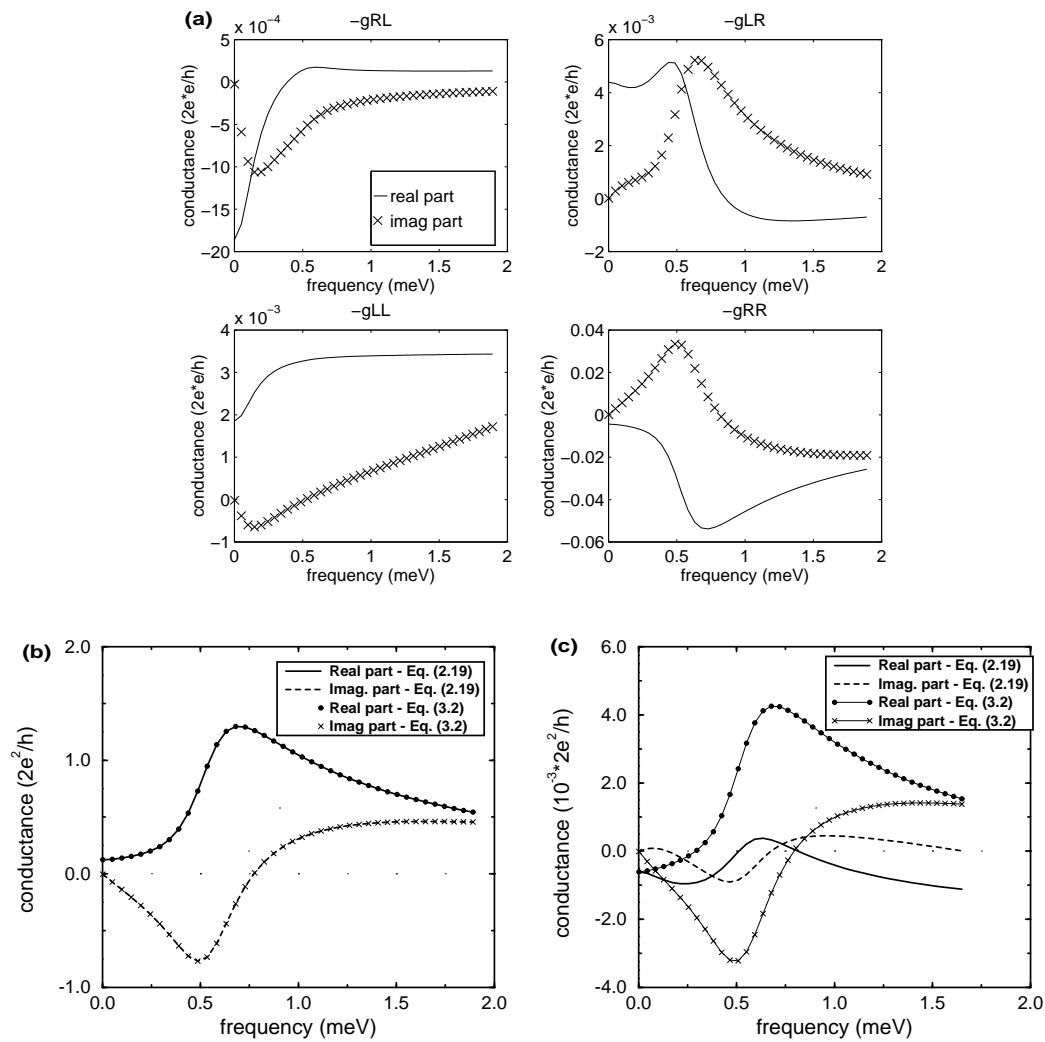


Fig. 4 / Anantram